

Mustafa Odabaşoğlu<sup>a\*</sup> and  
Orhan Büyükgüngör<sup>b</sup><sup>a</sup>Department of Chemistry, Faculty of Arts & Science, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey, and <sup>b</sup>Department of Physics, Faculty of Arts & Science, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey

Correspondence e-mail: muodabas@omu.edu.tr

## Key indicators

Single-crystal X-ray study  
*T* = 296 K  
Mean  $\sigma$ (C–C) = 0.003 Å  
*R* factor = 0.050  
*wR* factor = 0.133  
Data-to-parameter ratio = 13.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.3-(4-Fluoroanilino)isobenzofuran-1(3*H*)-oneCrystals of the title compound, C<sub>14</sub>H<sub>10</sub>FNO<sub>2</sub>, show paired N–H···O hydrogen bonds that link the molecules into *R*<sub>2</sub><sup>2</sup>(12) dimers; the hydrogen-bonded dimers are linked into chains by an aromatic  $\pi$ – $\pi$  stacking interaction.Received 17 July 2006  
Accepted 12 August 20063-Substituted phthalides,  
Part XIII

## Comment

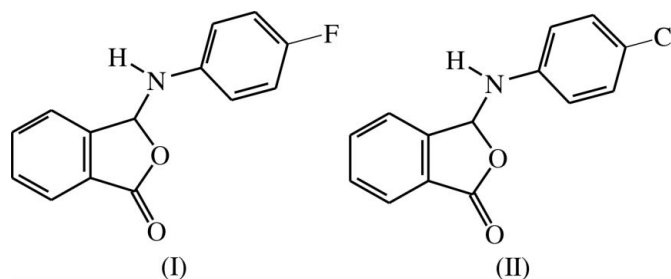
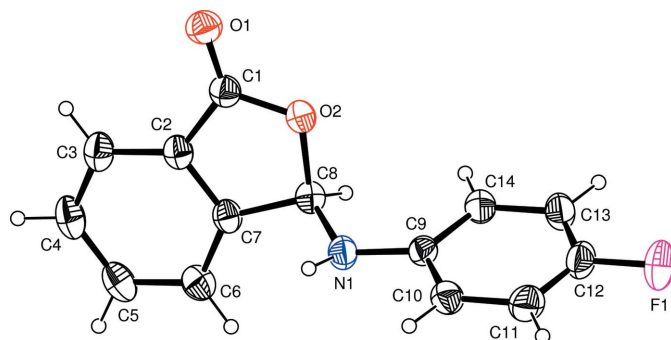
We report here the structure of 3-(4-fluoroanilino)isobenzofuran-1(3*H*)-one, (I) (Fig. 1 and Table 1), and briefly compare this with the structure of the chloro analogue, (II), which has been reported recently (Büyükgüngör & Odabaşoğlu, 2006). Compound (I) was prepared in a similar manner to compound (II), by reaction of phthalaldehydic acid and 4-fluoroaniline as starting materials. The dihedral angle between the *p*-fluorophenyl ring and the mean plane of the phthalide group is 74.10 (9)°; the analogous angle in (II) is 75.60 (15)°.The phthalide group (C1–C8/O2) is essentially planar, the largest deviation from the mean plane being 0.039 (2) Å for atom C8. The crystal packing is stabilized by intermolecular N–H···O hydrogen bonds (Fig. 2 and Table 1), which generate a dimeric *R*<sub>2</sub><sup>2</sup>(12) ring motif (Etter, 1990); hydrogen-bonded dimers are linked into chains by an aromatic  $\pi$ – $\pi$  stacking interaction (Fig. 3). The  $\pi$ ··· $\pi$  interaction occurs

Figure 1

A view of (I), showing the atomic numbering scheme, with displacement ellipsoids drawn at the 30% probability level.

between the two six-membered rings of the phthalide part at  $(-x, -y, 1 - z)$ , with a centroid-to-centroid distance of 3.6294 (13) Å and a plane-to-plane separation of 3.469 Å. Compound (II) has similar N—H···O hydrogen bonds and a  $\pi$ – $\pi$  stacking interaction but does not have a dimeric motif.

## Experimental

The title compound was prepared as described by Odabaşoğlu & Büyükgüngör (2006), using phthalaldehydic acid and 4-fluoroaniline as starting materials (yield 85%; m.p. 461–462 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a DMF solution at room temperature.

### Crystal data

$C_{14}H_{10}FNO_2$	$V = 559.71 (11) \text{ \AA}^3$
$M_r = 243.23$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.443 \text{ Mg m}^{-3}$
$a = 7.0041 (8) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.1023 (9) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$c = 10.2114 (12) \text{ \AA}$	$T = 296 \text{ K}$
$\alpha = 91.433 (9)^\circ$	Prism, colorless
$\beta = 93.906 (9)^\circ$	$0.48 \times 0.24 \times 0.11 \text{ mm}$
$\gamma = 104.300 (9)^\circ$	

### Data collection

Stoe IPDS-2 diffractometer	7292 measured reflections
$\omega$ scans	2202 independent reflections
Absorption correction: integration ( <i>X-RED32</i> ; Stoe & Cie, 2002)	1475 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.963$ , $T_{\max} = 0.988$	$R_{\text{int}} = 0.086$
	$\theta_{\max} = 26.0^\circ$

### Refinement

Refinement on $F^2$	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.050$	$w = 1/[\sigma^2(F_o^2) + (0.0718P)^2]$
$wR(F^2) = 0.133$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\max} < 0.001$
2202 reflections	$\Delta\rho_{\max} = 0.16 \text{ e \AA}^{-3}$
167 parameters	$\Delta\rho_{\min} = -0.18 \text{ e \AA}^{-3}$

**Table 1**

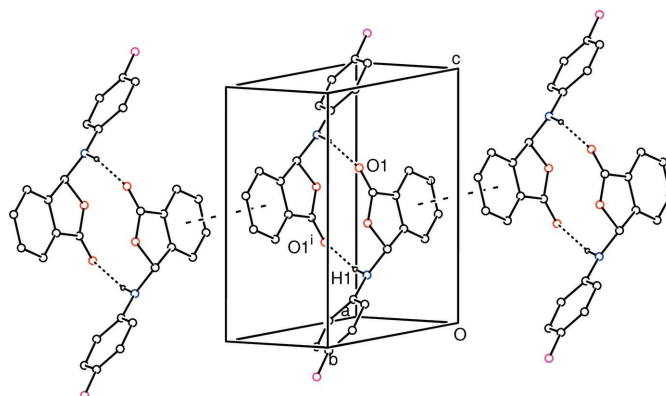
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots O1^i$	0.85 (2)	2.25 (2)	3.082 (2)	166.2 (18)

Symmetry code: (i)  $-x + 1, -y + 1, -z + 1$ .

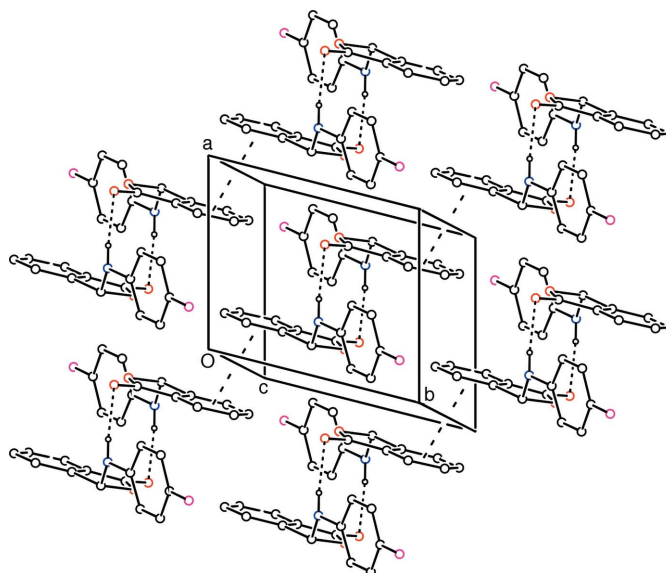
All H atoms attached to C atoms were treated as riding on their parent atoms, with C—H = 0.93 Å for aromatic and 0.98 Å for methine H atoms, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The H atom of the amino group was located in a Fourier difference map and freely refined.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).



**Figure 2**

Part of the crystal structure of (I), showing the formation of a hydrogen-bonded (dashed lines) dimer. For the sake of clarity, H atoms bonded to C atoms have been omitted. [Symmetry code: (i)  $1 - x, 1 - y, 1 - z$ ].



**Figure 3**

A packing diagram for (I), showing the N—H···O and  $\pi$ – $\pi$  interactions as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity.

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